

Free fermions and spin chains

Mapping spin models onto models of free fermions is a powerful tool in condensed matter. Here we will explore a mapping from quantum spins to fermions in two different cases: the XY spin chain and the transverse field Ising model. The utility of our mapping stems from the fact that Hamiltonians describing free particles, be they fermions or bosons, are exactly diagonalizable. We will use these examples to better understand second quantization, which allows us to build antisymmetry requirements of the wavefunction into our representation of a quantum state.

To begin, we examine what it means to map any model onto a model of fermions (or bosons — though the rest of the discussion will focus on the mapping to fermions). The key property of a quantum many-body wavefunction is the commutation/anticommutation properties determined by the properties of the particles described by the wavefunction. Often, when many-body wavefunctions are introduced, these requirements are enforced by writing the many-body wavefunction as a Slater determinant/permanent of a matrix of single-particle wavefunctions. However the resulting expressions are at best cumbersome to work with, and at worst totally intractable. In the *second quantized* formalism, we build these requirements of symmetry/antisymmetry of the wavefunction into its definition.

When we specify a quantum state, we do so by building up our state from the vacuum state with the application of creation operators at various quantum numbers (which could indicate position, momentum, etc). These creation operators, and their adjoints, the annihilation operators, can be constructed such that the many-body wavefunctions that they construct automatically satisfy the symmetry/antisymmetry requirements under exchange of particles (for bosons and fermions respectively). What are the requirements that these operators must satisfy in order to produce states with the desired properties? For bosons, the state is symmetric under the exchange of any pair of particles, and therefore the creation and annihilation operators commute except when creation and annihilation is done at the same site. For fermions, by contrast, antisymmetry is the norm and therefore creation and annihilation operators *anticommute* except when applied at the same site. Therefore if we have creation and annihilation operators c_i and c_i^\dagger , where i is a spatial index, then the bosonic commutation relations are

$$[c_i, c_j] = 0; \quad [c_i^\dagger, c_j^\dagger] = 0; \quad [c_i, c_j^\dagger] = \delta_{ij}, \quad (1)$$

while for fermions the anticommutation relations are

$$\{c_i, c_j\} = 0; \quad \{c_i^\dagger, c_j^\dagger\} = 0; \quad \{c_i, c_j^\dagger\} = \delta_{ij}, \quad (2)$$

where the square brackets represent commutation $[A, B] = AB - BA$ and the curly brackets represent anticommutation $\{A, B\} = AB + BA$.

1 Jordan Wigner Transformation

For the rest of these notes we will be working with spin $\frac{1}{2}$ particles, for which the spin operators in the x , y and z directions are respectively

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (3)$$

1.1 Single spin

Let us now consider a single spin- $\frac{1}{2}$ degree of freedom. We will work as usual in the z basis so that our basis vectors are

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (4)$$

which have eigenvalues of σ^z of ± 1 respectively. The insight of Jordan and Wigner is that we can think of spin up as being a site occupied by a fermion, and spin down as being an empty site. Then we can construct any basis state by repeated application of creation operators at different sites on the state of all spins down.

Conveniently, we can explicitly write down a representation of these creation operators for a single spin as

$$f = \frac{1}{2}(\sigma^x - i\sigma^y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}; \quad f^\dagger = \frac{1}{2}(\sigma^x + i\sigma^y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \quad f^\dagger f = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (5)$$

The creation operators can then be defined as $c = f$, $c^\dagger = f^\dagger$. Then one can explicitly check that $\{c, c\} = \{c^\dagger, c^\dagger\} = 0$ and $\{c, c^\dagger\} = 1$. Therefore these operators are fermionic operators. The operators f and f^\dagger are known as spin lowering and raising operators respectively and sometimes denoted by S^- and S^+ .

1.2 Multiple spins

One can now extend this picture to multiple spins. In this case we need to define creation operators acting on a particular spin, say at position i . The temptation would be to define $c_i = f_i$, $c_i^\dagger = f_i$, in analogy with the previous definition for a single spin. However, the spin lowering/raising operators *are not fermionic operators*. In particular, they commute rather than anticommute at different sites. However, we can define creation and annihilation operators c and c^\dagger which obey canonical fermion anticommutation relations, in terms of the spin operators. The intuition is as follows: currently f_i and f_j commute for $i \neq j$ because f_i is acting with the identity at site j and f_j is acting with the identity at site i , and the f 's commute with the identity. If we want them to anticommute, we need to attach to f_j an operator acting at site i that anticommutes with f_i , or vice versa

What is such an operator? Check that $e^{i\pi f^\dagger f}$ anticommutes with f . Then the idea that Jordan and Wigner had was the following: append to f_i a string of $e^{i\pi f^\dagger f}$'s acting on all the sites to the left of i . Then, for any $i < j$ (without loss of generality), there will be an $e^{i\pi f^\dagger f}$ acting on site i from c_j , and therefore c_i and c_j will anticommute! Therefore we have

$$c_i = \exp \left[i\pi \sum_{j < i} f_j^\dagger f_j \right] f_i; \quad c_i^\dagger = f_i^\dagger \exp \left[-i\pi \sum_{j < i} f_j^\dagger f_j \right]. \quad (6)$$

Note that $e^{i\pi f^\dagger f}$ is proportional to σ^z , as one can see from expanding out the form of $f^\dagger f$, which is a diagonal matrix and can be exponentiated easily. This transformation can be inverted since we have $c_i^\dagger c_i = f_i^\dagger f_i$. In particular we have

$$f_i = \exp \left[i\pi \sum_{j < i} c_j^\dagger c_j \right] c_i; \quad f_i^\dagger = c_i^\dagger \exp \left[-i\pi \sum_{j < i} c_j^\dagger c_j \right]. \quad (7)$$

These operators c_i are known as *Dirac fermions*. The ordering of the operators in the definition of c_i and c_i^\dagger is important, since fermionic operators *do not commute, even at different sites* (they anticommute).

2 XY spin chain

2.1 Fermionization

We have shown that one can construct fermionic creation and annihilation operators out of spin operators — though these fermionic operators are highly nonlocal in the spin operators. Therefore, any fermionic Hamiltonian written in terms of creation and annihilation operators can be rewritten as a nonlocal Hamiltonian of a spin- $\frac{1}{2}$ chain, and any spin- $\frac{1}{2}$ one dimensional Hamiltonian can be written in terms of fermionic operators.

How do we do this in an explicit example? Consider the Hamiltonian of a 1D lattice of spin $\frac{1}{2}$ particles with magnetic interactions in both the X and Y directions:

$$H = J_x \sum_i \sigma_i^x \sigma_{i+1}^x + J_y \sum_i \sigma_i^y \sigma_{i+1}^y. \quad (8)$$

Throughout, we will be cavalier about boundary conditions and assume translation invariance. Periodic boundary conditions actually introduce an extra term into the Jordan-Wigner transform of this Hamiltonian, but this term does not contribute in the infinite-system limit, and we will not deal with it here.

In terms of $f = \frac{1}{2}(\sigma^x - i\sigma^y)$ and $f^\dagger = \frac{1}{2}(\sigma^x + i\sigma^y)$, we can write this Hamiltonian as

$$H = J_x \sum_i (f_i + f_i^\dagger)(f_{i+1} + f_{i+1}^\dagger) - J_y \sum_i (f_i^\dagger - f_i)(f_{i+1}^\dagger - f_{i+1}), \quad (9)$$

which simplifies [remembering that the f 's commute at different sites!] to

$$H = (J_x - J_y) \sum_i [f_i f_{i+1} + f_{i+1}^\dagger f_i^\dagger] + (J_x + J_y) \sum_i [f_i^\dagger f_{i+1} + f_{i+1}^\dagger f_i]. \quad (10)$$

We can then write the lowering and raising operators f in terms of fermionic operators, in order to get

$$H = (J_x - J_y) \sum_i c_i e^{i\pi n_i} c_{i+1} + (J_x + J_y) \sum_i c_i^\dagger e^{i\pi n_i} c_{i+1} + \text{h.c.} \quad (11)$$

where we have introduced $n_i = c_i^\dagger c_i$, the number operator. Now we can use the fact that $e^{\pm i\pi n_i} = 1 - 2f_i^\dagger f_i = 1 - 2c_i^\dagger c_i$, which can be seen from the explicit matrix form of f above. Note that the n_i commute with all operators at different

sites, since the two minus signs obtained from commuting an n_i past a fermionic operator cancel. Substituting this in above and commuting operators past each other so that we can cancel c_i^2 and $(c_i^\dagger)^2$, which both vanish, we obtain a minus sign on the term proportional to $J_x - J_y$, which we can absorb by commuting c_i and c_{i+1} at the expense of a minus sign. Then our Hamiltonian in terms of fermion operators is

$$H = (J_x - J_y) \sum_i c_{i+1} c_i + (J_x + J_y) \sum_i c_i^\dagger c_{i+1} + \text{h.c.} \quad (12)$$

Note that this Hamiltonian does not conserve total particle number: it does not commute with $\sum_i c_i^\dagger c_i$ because of the terms proportional to $J_x - J_y$. [As an exercise, show explicitly that $c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i$ commutes with $c_i^\dagger c_i + c_{i+1}^\dagger c_{i+1}$, but $c_i c_{i+1} + c_{i+1}^\dagger c_i^\dagger$ does not.] However in the isotropic case $J_x = J_y = J/2$, then we obtain

$$H = J \sum_i c_i^\dagger c_{i+1} + \text{h.c.} \quad (13)$$

This Hamiltonian does conserve particle number. Although it is not necessary to conserve particle number in order to diagonalize a free fermionic Hamiltonian, for now we will work in the isotropic case, since things are a bit simpler. Note that our Hamiltonian is free fermionic in the sense that it is quadratic in fermionic operators — this means that the Hamiltonian does not have interactions but only hopping between different sites.

2.2 Fourier transformation of isotropic model

For now we see that our model has the form

$$H = J \sum_{i,j} c_i^\dagger A_{ij} c_j, \quad (14)$$

where A_{ij} depends only on $|i - j|$: in particular $A_{ij} = \delta_{|i-j|,1}$. This translation invariance should be alerting us to the utility of Fourier transformation, which we can use to move to a basis where A is diagonal, so that we can write our Hamiltonian as

$$H = J \sum_k \epsilon_k \eta_k^\dagger \eta_k \quad (15)$$

for fermionic operators η_k which are linear combinations of the c_i . This would diagonalize the Hamiltonian in the occupation number basis, and allow us to read off the dispersion relation as ϵ_k as a function of wavenumber k .

Let us define the η as the Fourier transform of the c , so that

$$c_n = \sum_k e^{ikR_n} \eta_k; \quad \eta_k = \sum_n e^{-ikR_n} c_n. \quad (16)$$

Then we can see that the Hamiltonian can be rewritten as

$$H = J \sum_{n,m,k,k'} \left[e^{ikR_n - ik'R_m} \eta_k^\dagger \eta_{k'} A_{nm} \right]. \quad (17)$$

Using the fact that $A_{nm} = \delta_{|n-m|,1}$, and doing the sum over n and m while assuming that the lattice constant is $R_{n+1} - R_n = a$, we have

$$H = J \sum_{k,k',n} \left[e^{ikR_n - ik'(R_n+a)} + e^{ik(R_n+a) - ik'R_n} \right] \eta_k^\dagger \eta_{k'}. \quad (18)$$

By doing the sum over n , we get a delta function $\delta_{k,k'}$, and so our Hamiltonian can be written as

$$H = 2J \sum_k \epsilon_k \eta_k^\dagger \eta_k, \quad \epsilon_k = \cos(ka). \quad (19)$$

This tells us that the dispersion relation i.e. the energy of an excitation with wavenumber k is $2J \cos(ka)$. For a ferromagnet, with the way that we have defined the Hamiltonian, the J should be negative, and so for $|ka| < \pi/2$, excitations with wavevector k will reduce the energy of a state. The ground state is then the state that we get by applying all these energy-reducing operators to the vacuum state. The corresponding ground state energy density is

$$E_{gs} = \frac{2J}{L} \sum_{|k| < \pi/2a} \epsilon_k \approx 2J \int_{-\pi/2}^{\pi/2} \frac{d(ka)}{2\pi} \cos(ka). \quad (20)$$

The magnetization in the ground state is related to the number of fermions in the chain, since $n_i = \frac{1}{2}(1 + \sigma^z)$. Therefore the magnetization is $\frac{1}{L} \sum_i \sigma_i^z = \frac{2}{L} \sum_i n_i - 1$. Now we can calculate the magnetization in the ground state, by first calculating the fermion density N/L in the ground state:

$$\frac{N_{gs}}{L} = \frac{1}{L} \sum_{|k| < \pi/2a} 1 \approx \int_{-\pi/2}^{\pi/2} \frac{d(ka)}{2\pi} = \frac{1}{2}. \quad (21)$$

Therefore the magnetization in the ground state is $2 \times \frac{1}{2} - 1 = 0$.

2.3 Anisotropic chain

What about the case where $J_x \neq J_y$? In this case the Hamiltonian no longer commutes with $\sum_i n_i$ and therefore does not conserve particle number. Therefore the eigenstates of H cannot be written as a linear combination of creation operators acting on the vacuum state. To find the eigenstates of H we need to introduce another transformation which will make the form of these states clearer. We have

$$H = (J_x - J_y) \sum_i c_{i+1} c_i + (J_x + J_y) \sum_i c_i^\dagger c_{i+1} + \text{h.c.} \quad (22)$$

which we can write as

$$H = J \sum_i \left[c_i^\dagger c_{i+1} + \gamma c_{i+1} c_i \right] + \text{h.c.} \quad (23)$$

for $\gamma = \frac{J_x - J_y}{J}$ which is zero in the isotropic case $J_x = J_y$. Fourier transforming, we have

$$H = 2J \sum_k \cos(ka) \eta_k^\dagger \eta_k + \gamma J \sum_k \left(e^{-ika} \eta_k \eta_{-k} + e^{ika} \eta_{-k}^\dagger \eta_k^\dagger \right). \quad (24)$$

To make things look more symmetrical, we can sum over only positive k , and write

$$H = 2J \sum_{k>0} \cos(ka) (\eta_k^\dagger \eta_k + \eta_{-k}^\dagger \eta_{-k}) + 2i\gamma J \sum_{k>0} \sin(ka) (\eta_{-k} \eta_k - \eta_k^\dagger \eta_{-k}^\dagger). \quad (25)$$

However, due to the presence of the terms which break particle number conservation, this Hamiltonian is not diagonal. In order to diagonalize this Hamiltonian we have to make what is called a Bogoliubov transformation; which involves rotation c and c^\dagger into each other, defining new creation and annihilation operators as linear combinations of c and c^\dagger such that canonical fermionic anticommutation is still satisfied, but our Hamiltonian is now diagonal.

2.4 The Bogoliubov transformation

The Bogoliubov transformation can be illustrated with a generic free fermionic (i.e. quadratic) Hamiltonian which does not conserve particle number. The transformation consists of rotating creation and annihilation operators into each other in order to diagonalize the Hamiltonian. Let us consider a particular term in the Hamiltonian with the form

$$H = \Omega(a^\dagger a + b^\dagger b) + \lambda(a^\dagger b^\dagger + ba), \quad (26)$$

where Ω is coefficient for the diagonal piece and λ is the coefficient for the off-diagonal piece. We define transformed operators α and β according to

$$a = u\alpha - v\beta^\dagger \quad (27)$$

$$b = u\beta + v\alpha^\dagger, \quad (28)$$

where u and v are complex numbers that we will choose in order to make our transformation useful. We will assume that α and β obey canonical fermion anticommutation relations. Therefore, in order for the α and β to obey canonical anticommutation relations, we need $|u|^2 + |v|^2 = 1$. Let us assume that u and v are real — then we can parameterize them as $u = \cos(\theta/2)$ and $v = \sin(\theta/2)$, which gives

$$a = \cos(\theta/2)\alpha - \sin(\theta/2)\beta^\dagger \quad (29)$$

$$b = \cos(\theta/2)\beta + \sin(\theta/2)\alpha^\dagger. \quad (30)$$

We can plug these into the Hamiltonian and use fermionic commutation relations to find, after some algebra, that

$$H = 2\Omega \sin^2(\theta/2) - \lambda \sin \theta + (\Omega \cos \theta + \lambda \sin \theta)(\alpha^\dagger \alpha + \beta^\dagger \beta) + (\lambda \cos \theta - \Omega \sin \theta)(\alpha^\dagger \beta^\dagger + \beta \alpha). \quad (31)$$

Now we would like to choose θ so that the off-diagonal part, proportional to $\alpha^\dagger \beta^\dagger + \beta \alpha$, vanishes. Therefore we should choose $\tan \theta = \lambda/\Omega$. With this choice, $\sin \theta = \lambda/\sqrt{\lambda^2 + \Omega^2}$ and $\cos \theta = \Omega/\sqrt{\lambda^2 + \Omega^2}$, and $\sin^2 \frac{\theta}{2} = \frac{1}{2}(1 - \Omega/\sqrt{\lambda^2 + \Omega^2})$. Therefore our Hamiltonian becomes

$$H = \Omega - \sqrt{\lambda^2 + \Omega^2} + \sqrt{\lambda^2 + \Omega^2}(\alpha^\dagger \alpha + \beta^\dagger \beta). \quad (32)$$

We will now proceed to use this formula to diagonalize the XY spin chain.

2.5 Back to the anisotropic XY chain

Identifying the terms in equation 25 with the form in equation 26, we see that

$$\Omega = 2J \cos(ka), \quad \lambda = 2\gamma J \sin(ka), \quad a = e^{i\pi/4} \eta_k, \quad b = e^{i\pi/4} \eta_{-k}. \quad (33)$$

Therefore we must choose $\tan \theta = \gamma \tan(ka)$. If we introduce the rotated creation and annihilation operators ξ_k and ξ_{-k} , defined according to equation 29, then we find a Hamiltonian

$$H = \sum_{k>0} 2J \left[\cos(ka) - \epsilon_k + \epsilon_k (\xi_k^\dagger \xi_k + \xi_{-k}^\dagger \xi_{-k}) \right], \quad \epsilon_k = \sqrt{\gamma^2 \sin^2(ka) + \cos^2(ka)}. \quad (34)$$

Since $\epsilon_k = \epsilon_{-k}$, we can rewrite this as

$$H = E_0 + 2J \sum_k \epsilon_k \xi_k^\dagger \xi_k, \quad (35)$$

where E_0 is just a constant shift given by $2J \sum_{k>0} (\cos(ka) - \epsilon_k)$.

Since the dispersion ϵ_k is always positive, we know that the ground state has to be the vacuum, since there are no operators which will lower the energy of the vacuum. However, note that the vacuum in this transformed basis is *not the same* as the vacuum in the original η basis. In particular, the magnetization (related to the expectation of the η number operator) may be nonzero even if the state is the vacuum of the ξ basis.

3 Transverse field Ising model

Now consider a different model Hamiltonian: the transverse field Ising chain. Here there is a coupling in the z component of spins at neighboring sites, and there is a transverse field in the x direction that destroys order in the z direction if it is strong enough. In fact, the ordering transition as the strength of the transverse field decreases is the same as that of the 2 dimensional classical Ising model, and in fact it is often simpler to study the critical properties of the quantum model, as we will do here. The Hamiltonian is

$$H = J \sum_i \sigma_i^x \sigma_{i+1}^x + h \sum_i \sigma_i^z \quad (36)$$

$$= J \sum_i (f_i + f_i^\dagger)(f_{i+1} + f_{i+1}^\dagger) + h \sum_i \sigma_i^z. \quad (37)$$

Writing the spin Hamiltonian in terms of the fermion operators c and c^\dagger , we find that

$$H = J \sum_j \left[c_j e^{i\pi n_j} c_{j+1} + c_j^\dagger e^{i\pi n_j} c_{j+1}^\dagger + c_j^\dagger e^{i\pi n_j} c_{j+1} + c_j e^{i\pi n_j} c_{j+1}^\dagger \right] + h \sum_i (1 - 2c_i^\dagger c_i). \quad (38)$$

Note that we can write the Hamiltonian as

$$H = J \sum_n [c_n^\dagger c_{n+1} + c_n c_{n+1}] + h \sum_i \left[\frac{1}{2} - c_n^\dagger c_n \right] + \text{h.c.} \quad (39)$$

This Hamiltonian does not conserve particle number because of the term $c_n c_{n+1}$ and its conjugate. However, it does preserve *parity* of particle number, since particles are always created or annihilated in pairs.

As before, we need to Fourier transform in order to diagonalize this Hamiltonian. Doing out the Fourier transform as before, defining η_k as the Fourier transform of the c_n , we find that

$$H = \sum_k \left[(-2h + 2J \cos(ka)) \eta_k^\dagger \eta_k + J(e^{-ika} \eta_k \eta_{-k} + e^{ika} \eta_{-k}^\dagger \eta_k^\dagger) \right]. \quad (40)$$

As before, we can write this Hamiltonian more symmetrically as

$$H = \sum_{k>0} \left[(2J \cos(ka) - 2h)(\eta_k^\dagger \eta_k + \eta_{-k}^\dagger \eta_{-k}) + 2iJ \sin(ka)(\eta_{-k} \eta_k - \eta_k^\dagger \eta_{-k}^\dagger) \right]. \quad (41)$$

This Hamiltonian is now in a form where we can do the Bogoliubov transformation as we did for the XY chain above. Identifying the terms in equation 41 with the form in equation 26, we see that

$$\Omega = 2J \cos(ka) - 2h, \quad \lambda = 2J \sin(ka), \quad a = e^{i\pi/4} \eta_k, \quad b = e^{i\pi/4} \eta_{-k}. \quad (42)$$

Using $\Omega = 2J \cos(ka) - 2h$ and $\lambda = 2J \sin(ka)$, we the Bogoliubov-transformed Hamiltonian

$$H = \sum_{k>0} 2J \left[\cos(ka) - \frac{h}{J} - \epsilon_k + \epsilon_k (\xi_k^\dagger \xi_k + \xi_{-k}^\dagger \xi_{-k}) \right], \quad \epsilon_k = \pm \sqrt{1 - 2h/J \cos ka + (h/J)^2}. \quad (43)$$

Plotting this dispersion relation, one sees that there are two bands of excitations, and the band gap between them closes at $h = J$, which is the critical point of the transverse field Ising model. If we want to calculate the energy of the ground state, then we can integrate the negative branch of the dispersion relation over the Brillouin zone for k from $-\pi$ to π , since the negative branch remains negative over the whole Brillouin zone. The ground state energy density is given by

$$E_{gs} = -2J \int_{-\pi}^{\pi} \frac{d(ka)}{2\pi} \sqrt{1 - 2h/J \cos ka + (h/J)^2}. \quad (44)$$

Note that this is different from the free energy of the 2D classical Ising model. However in the appropriate anisotropic limit of the 2D classical model, one should recover this form of the free energy, as we discuss in another set of notes on quantum – classical mappings. For now we will state that the critical properties of the transverse field Ising model

4 References

[Notes by GT Landi](#)

[Notes by Max Metlitski](#)